



# 1+1+1 Flavor QCD+QED Simulation at the Physical Point

Y.Kuramashi (U. of Tsukuba/RIKEN AICS)  
for PACS-CS Collaboration

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## Collaboration members

### • Physicists:

S.Aoki, N.Ishizuka, K.Kanaya, Y.Kuramashi, Y.Namekawa, Tsukuba  
Y.Taniguchi, A.Ukawa, N.Ukita, T.Yamazaki, T.Yoshie

K.-I.Ishikawa, M.Okawa Hiroshima

D.Kadoh, Y.Nakamura, T.Izubuchi RIKEN

### • Computer scientists:

T.Boku, M.Sato, D.Takahashi, O.Tatebe Tsukuba  
T.Sakurai, H.Tadano



## Plan of talk

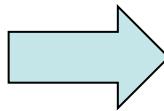
- §1. Introduction
- §2. Previous works
- §3. Method
- §4. Parameters and solver
- §5. Results
- §6. Summary



## §1. Introduction

Isospin symmetry breaking

- Quark mass difference:  
 $m_u \neq m_d$
- Electric charge difference  
 $e_{ph} Q_u \neq e_{ph} Q_d, e_{ph}^2 = 4\pi/137$



Mass splittings among isospin multiplets

$$m_{\pi^0} - m_{\pi^\pm}, m_{K^0} - m_{K^\pm}, m_n - m_p$$

1+1+1 flavor QCD+QED simulation is a straightforward way

isospin multiplets  $\Leftrightarrow$  u,d,s quark masses



## §2. Previous works

Group	Ref	Action
Duncan et al.	PRL76(1996)3896	qQED+qQCD Wilson
Blum et al.	PRD76(2007)114508	qQED+Nf=2 QCD DW
Blum et al.	PRD82(2010)094508	qQED+Nf=2+1 QCD DW
MILC	Lat08,Lat10	qQED+Nf=2+1 QCD Stag
BMW	Lat10	qQED+Nf=2+1 QCD Clover
Duncan et al.	PRD71(2005)094509	Test of RW for fQED DW
Ishikawa et al.	arXiv:1202.6018	fQED+Nf=2+1 QCD DW RW for fQED



### §3. Method

Reweighting from Nf=2+1 QCD to Nf=1+1+1 QCD+QED

$$\langle \mathcal{O}[U](\kappa_u^*, \kappa_d^*, \kappa_s^*) \rangle_{(\kappa_u^*, \kappa_d^*, \kappa_s^*), \text{fQED}} = \frac{\langle \mathcal{O}[U](\kappa_u^*, \kappa_d^*, \kappa_s^*) \det[W_{uds}[U]] \rangle_{(\kappa_{ud}, \kappa_s), \text{qQED}}}{\langle \det[W_{uds}[U]] \rangle_{(\kappa_{ud}, \kappa_s), \text{qQED}}}$$

with  $(\kappa_u^*, \kappa_d^*, \kappa_s^*)$  hopping parameters at the physical point

$$W_{uds}[U] = \prod_{q=u,d,s} \frac{D(e_{\text{ph}} Q_q, \kappa_q^*)}{D(0, \kappa_q)}$$



## Evaluation of $\det[W_{uds}[U]]$

Introduce a complex bosonic field  $\eta$

$$|\det[W_{uds}]|^2 = \langle e^{-|W_{uds}^{-1}\eta|^2 + |\eta|^2} \rangle_\eta$$

Given a set of  $\eta_i$  ( $i=1, \dots, N_\eta$ ) with Gaussian distribution

$$\det[W_{uds}[U]] = \left[ \lim_{N_\eta \rightarrow \infty} \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} e^{-|W_{uds}^{-1}[U]\eta_i|^2 + |\eta_i|^2} \right]^{\frac{1}{2}}$$



# Reduction of fluctuations in stochastic evaluation

- Determinant breakup Hasenfratz et al., PRD78(2008)014515
- divide the reweighting path  $(e=0; \kappa_{ud}, \kappa_s) \Rightarrow (e=e_{ph}; \kappa_u^*, \kappa_d^*, \kappa_s^*)$
- in the parameter space into  $N_B$  subintervals

$$\det[W_{uds}] = \det[W_{uds}^{(1)}] \times \det[W_{uds}^{(2)}] \times \cdots \times \det[W_{uds}^{(N_B)}]$$

- Combined reweighting factor
  - Averaged photon field
- } explained in next slides



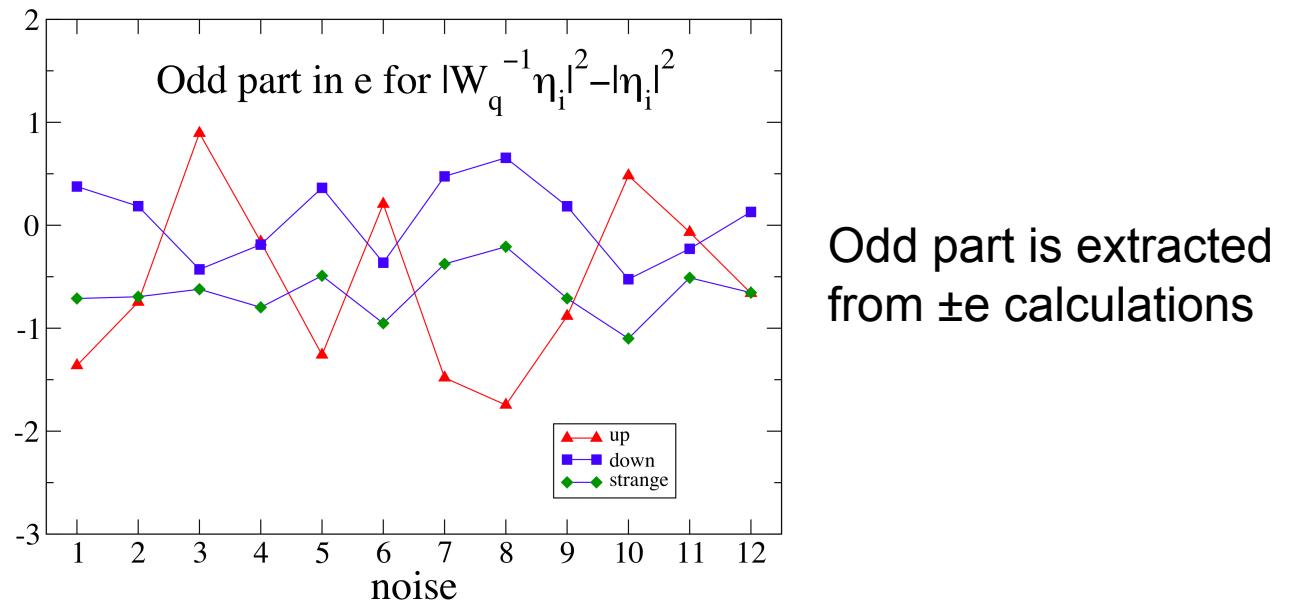
# Combined reweighting factor

Ishikawa et al., arXiv:1202.6018

- Combined reweighting factor for u,d,s quarks with a single set of noise

$$\det[W_{uds}[U]] = \left[ \lim_{N_\eta \rightarrow \infty} \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} e^{-|W_{uds}^{-1}[U]\eta_i|^2 + |\eta_i|^2} \right]^{\frac{1}{2}}$$

$\det[W_{uds}]$  rather than  $\det[W_u] \times \det[W_d] \times \det[W_s]$



Leading contribution of  $O(e)$  is partially cancelled due to  $Q_u + Q_d + Q_s = 0$



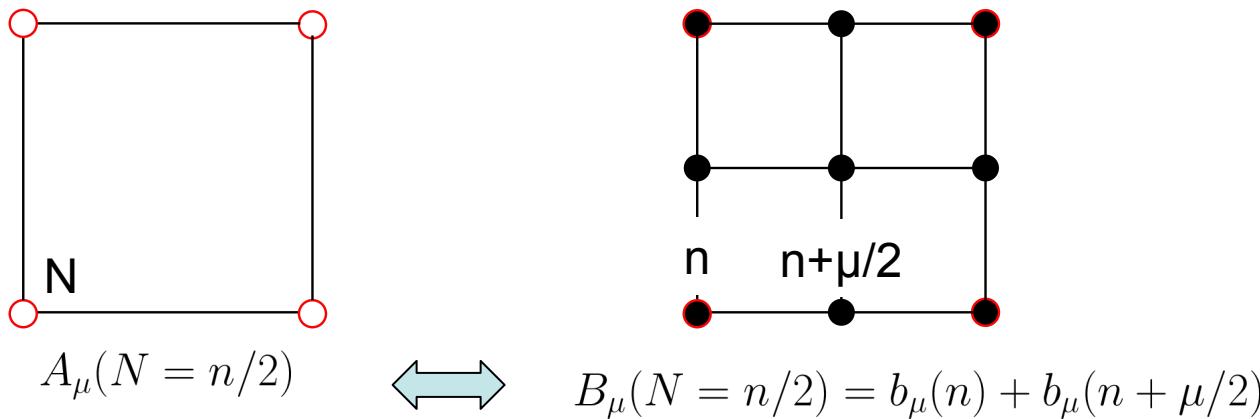
## Averaged photon field (1)

- generate photon field  $b_\mu$  on  $64^3 \times 128$  lattice ( $\Leftrightarrow 32^3 \times 64$  QCD lattice)  
with non-compact pure gauge action

$$S_b = \sum_{n,\mu,\nu} \frac{1}{4} (\partial_\mu b_\nu(n) - \partial_\nu b_\mu(n))^2 + \sum_{n,\mu,\nu} c_1 (\partial_\mu (\partial_\mu b_\nu(n) - \partial_\nu b_\mu(n)))^2$$

$c_1 = -0.646$  is chosen such that

$$\left\langle \sum_{N,\mu,\nu} \frac{1}{4} (\nabla_\mu A_\nu(N) - \nabla_\nu A_\mu(N))^2 \right\rangle = \left\langle \sum_{N,\mu,\nu} \frac{1}{4} (\nabla_\mu B_\nu(N) - \nabla_\nu B_\mu(N))^2 \right\rangle$$



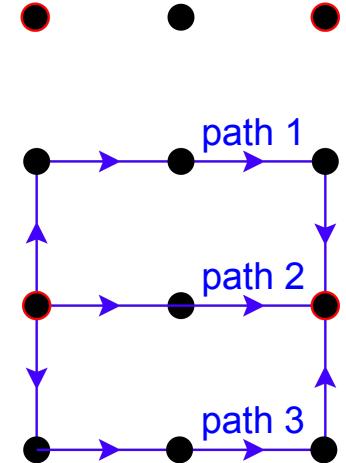
$$S_A = \sum_{N,\mu,\nu} \frac{1}{4} (\partial_\mu A_\nu(N) - \partial_\nu A_\mu(N))^2$$



## Averaged photon field (2)

- averaged photon fields over independent paths inside the  $2^4$  hypercube on the QED lattice

$$\begin{aligned}
 \bar{B}_\mu(N = n/2) = & \frac{1}{27} [(b_\mu(n) + b_\mu(n + \hat{\mu}/2)) \\
 & + \sum_{\nu \neq \mu} \sum_{\nu_s = \pm \nu} (b_{\nu_s}(n) + b_\mu(n + \hat{\nu}_s/2) + b_\mu(n + \hat{\nu}_s/2 + \hat{\mu}/2) - b_{\nu_s}(n + \hat{\mu})) \\
 & + \frac{1}{2} \sum_{\rho \neq \nu \neq \mu} \sum_{\rho_s = \pm \rho} \sum_{\nu_s = \pm \nu} (b_{\rho_s}(n) + b_{\nu_s}(n + \hat{\rho}_s/2) \\
 & \quad + b_\mu(n + \hat{\rho}_s/2 + \hat{\nu}_s/2) + b_\mu(n + \hat{\rho}_s/2 + \hat{\nu}_s/2 + \hat{\mu}/2) \\
 & \quad - b_{\rho_s}(n + \hat{\mu}) - b_{\nu_s}(n + \hat{\rho}_s/2 + \hat{\mu})) \\
 & + \frac{1}{6} \sum_{\sigma \neq \rho \neq \nu \neq \mu} \sum_{\sigma_s = \pm \sigma} \sum_{\rho_s = \pm \rho} \sum_{\nu_s = \pm \nu} (b_{\sigma_s}(n) + b_{\rho_s}(n + \hat{\sigma}_s/2) + b_{\nu_s}(n + \hat{\sigma}_s/2 + \hat{\rho}_s/2) \\
 & \quad + b_\mu(n + \hat{\sigma}_s/2 + \hat{\rho}_s/2 + \hat{\nu}_s/2) + b_\mu(n + \hat{\sigma}_s/2 + \hat{\rho}_s/2 + \hat{\nu}_s/2 + \hat{\mu}/2) \\
 & \quad - b_{\sigma_s}(n + \hat{\mu}) - b_{\rho_s}(n + \hat{\sigma}_s/2 + \hat{\mu}) - b_{\nu_s}(n + \hat{\sigma}_s/2 + \hat{\rho}_s/2 + \hat{\mu}))]
 \end{aligned}$$



- construct U(1) link variable in terms of the averaged photon field
- numerically checked that the averaged and conventional photon fields give consistent results for  $m_{PS0}-m_{PS\pm}$



## §4. Parameters and solver

- Configuration parameters PACS-CS, PRD81(2010)074503

$N_f=2+1$  flavor QCD near the physical point

NP O( $a$ )-improved Wilson-clover quark and Iwasaki gauge action

$\beta=1.9$ ,  $32^3 \times 64$ ,  $a \sim 0.1\text{fm}$ ,  $(\kappa_{ud}, \kappa_s) = (0.137785, 0.13660)$ , 2000 MD time

- Reweighting parameters

physical point:  $(\kappa_u^*, \kappa_d^*, \kappa_s^*) = (0.13787014, 0.13779700, 0.13669510)$

determined from  $\pi^+, K^+, K^0, \Omega^-$  masses

$$e_{ph}^2 = 4\pi/137$$

$N_B = 426$ ,  $N_\eta = 12$  for each piece of divided determinant

- Modified block BiCGStab Nakamura et al., CPC183(2012)34

quark matrix inversions for  $N_\eta = 12$  noises

a factor of  $3 \sim 4$  cost reduction compared with non-block solvers



## Modified block BiCGStab (1)

A solver algorithm for linear eqs with multiple right-hand sides

$$Dx^{(i)} = b^{(i)} \quad (i=1, \dots, L) \Rightarrow DX = B$$

```
1 initial guess  $X \in \mathbb{C}^{N \times L}$ 
2  $R = B - AX$ 
3  $P = R$ 
4 choose  $\tilde{R} \in \mathbb{C}^{N \times L}$ 
while  $\max_i(|r^{(i)}|/|b^{(i)}|) \leq \epsilon$ 
    4.1 QR decomposition  $P = Q\gamma, P \leftarrow Q$ 
    4.2  $U = MP$ 
    4.3  $V = AU$ 
    4.4 solve( $\tilde{R}^H V$ ) $\alpha = \tilde{R}^H R$  for  $\alpha$ 
    4.5  $T = R - V\alpha$ 
do {
    4.6  $S = MT$ 
    4.7  $Z = AS$ 
    4.8  $\zeta = \text{Tr}(Z_k^H T_k) / \text{Tr}(Z_k^H Z_k)$ 
    4.9  $X \leftarrow X + U\alpha + \zeta S$ 
    4.10  $R = T - \zeta Z$ 
    4.11 solve( $\tilde{R}^H V$ ) $\beta = -\tilde{R}^H Z$  for  $\beta$ 
    4.12  $P \leftarrow R + (P - \zeta V)\beta$ 
5 return ( $X$ )
```

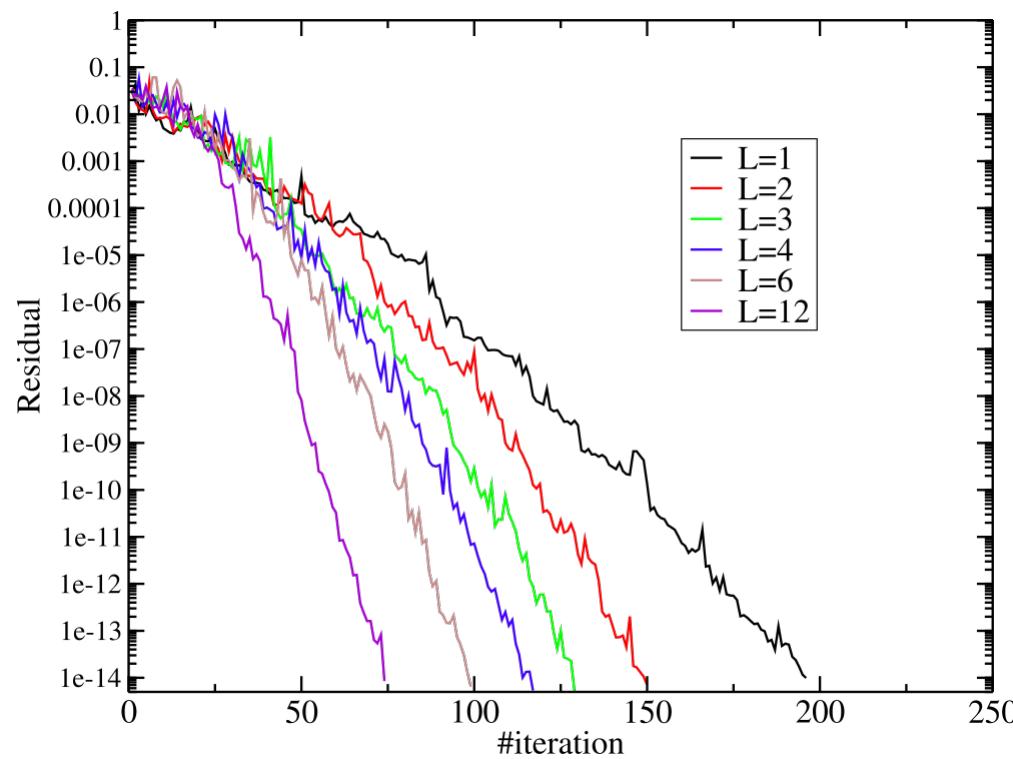
Basic idea: blocked version searches the solution vectors  
with the enlarged Krylov subspace



## Modified block BiCGStab (2)

a representative case

$N_f=2+1$  QCD,  $32^3 \times 64$ ,  $a \sim 0.1\text{fm}$ ,  
 $(\kappa_{ud}, \kappa_s) = (0.137785, 0.13660)$ , point source





## Modified block BiCGStab (3)

Performance test averaged over 10 configs

$$Dx^{(i)} = b^{(i)} \quad (i=1, \dots, 12)$$

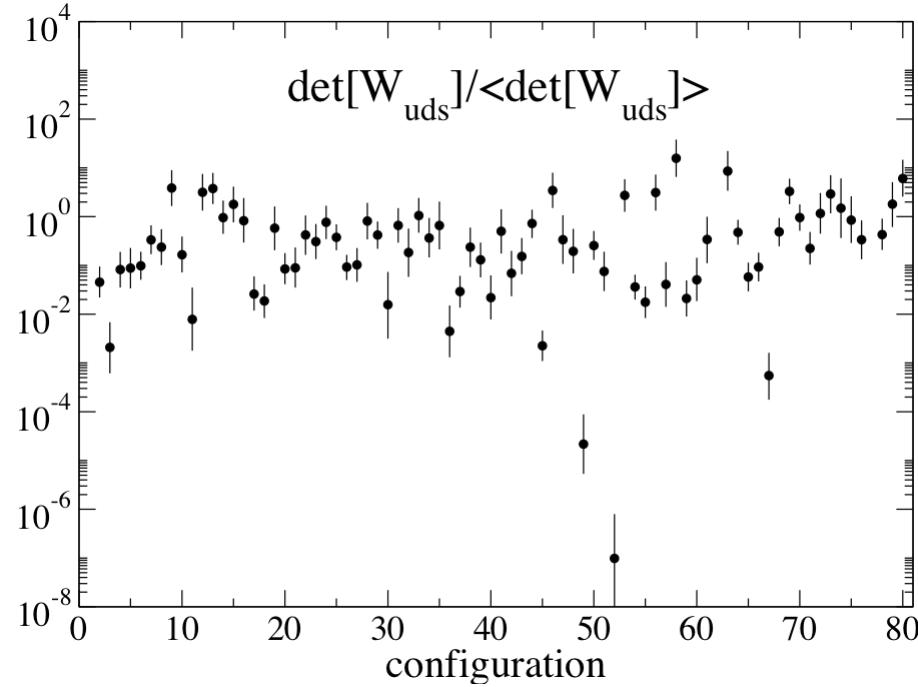
$L \times 12/L$	Time [s]	$T$ (gain)	NMVM	NM (gain)
$1 \times 12$	3827 (755)	1	17146 (3326)	1
$2 \times 6$	2066 (224)	1.9	12942 (1379)	1.3
$3 \times 4$	1619 (129)	2.4	10652 (832)	1.6
$4 \times 3$	1145 (99)	3.3	9343 (835)	1.8
$6 \times 2$	1040 (87)	3.7	7888 (663)	2.2
$12 \times 1$	705 (70)	5.4	6106 (633)	2.8

$T(\text{gain}) > NM(\text{gain})$  is thanks to effective usage of cache



## §5. Results

Configuration dependence of reweighting factor



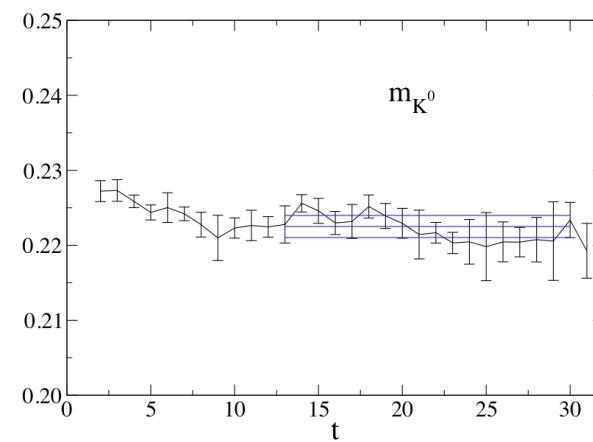
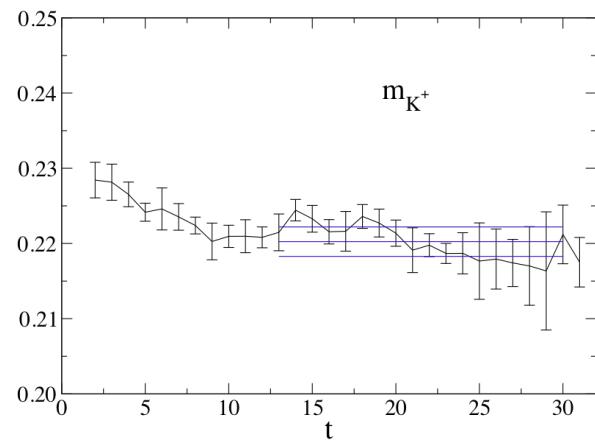
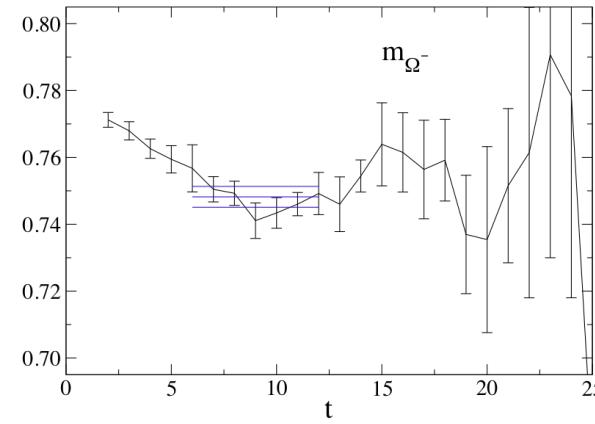
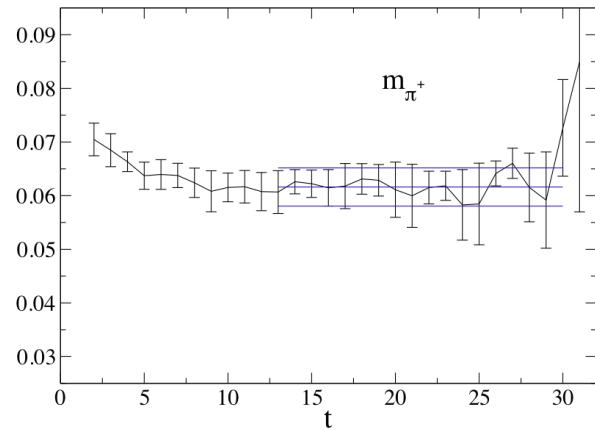
Normalized by  $\langle \det[W_{uds}] \rangle$

$$\langle \mathcal{O}[U](\kappa_u^*, \kappa_d^*, \kappa_s^*) \rangle_{(\kappa_u^*, \kappa_d^*, \kappa_s^*), \text{fQED}} = \frac{\langle \mathcal{O}[U](\kappa_u^*, \kappa_d^*, \kappa_s^*) \det[W_{uds}[U]] \rangle_{(\kappa_{ud}, \kappa_s), \text{qQED}}}{\langle \det[W_{uds}[U]] \rangle_{(\kappa_{ud}, \kappa_s), \text{qQED}}}$$



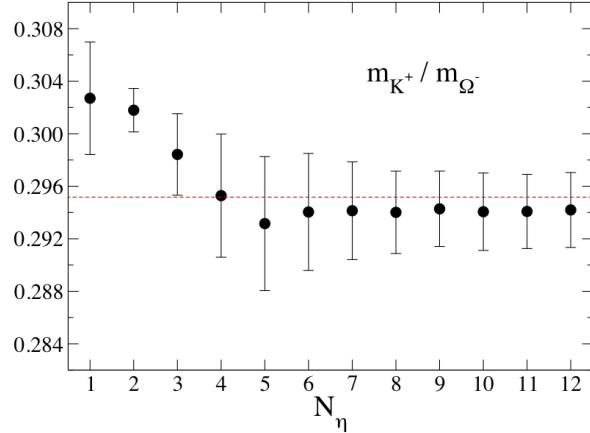
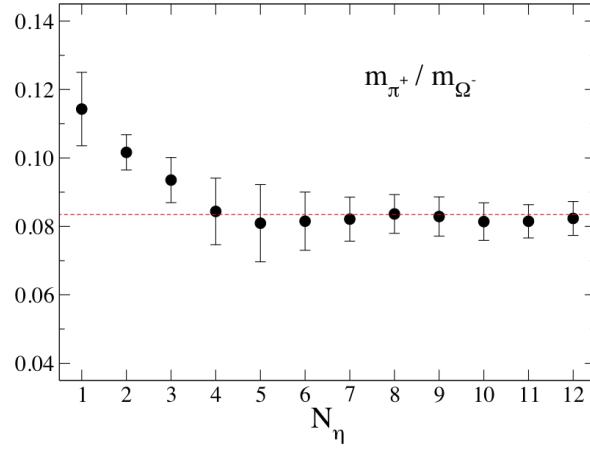
# Effective masses for $\pi^+, K^+, K^0, \Omega^-$

Smear-local propagators,  $N_\eta=12$

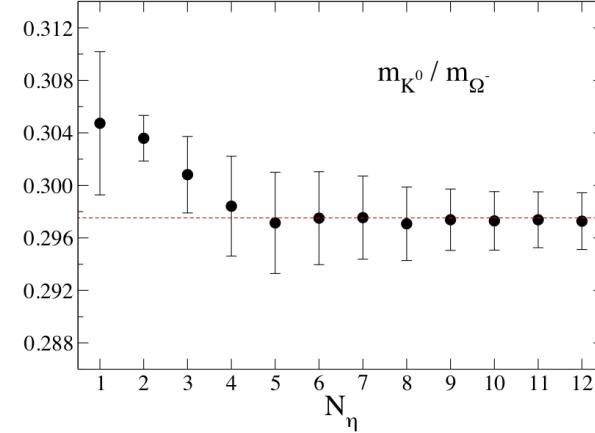




## $N_\eta$ dependence of hadron mass ratios



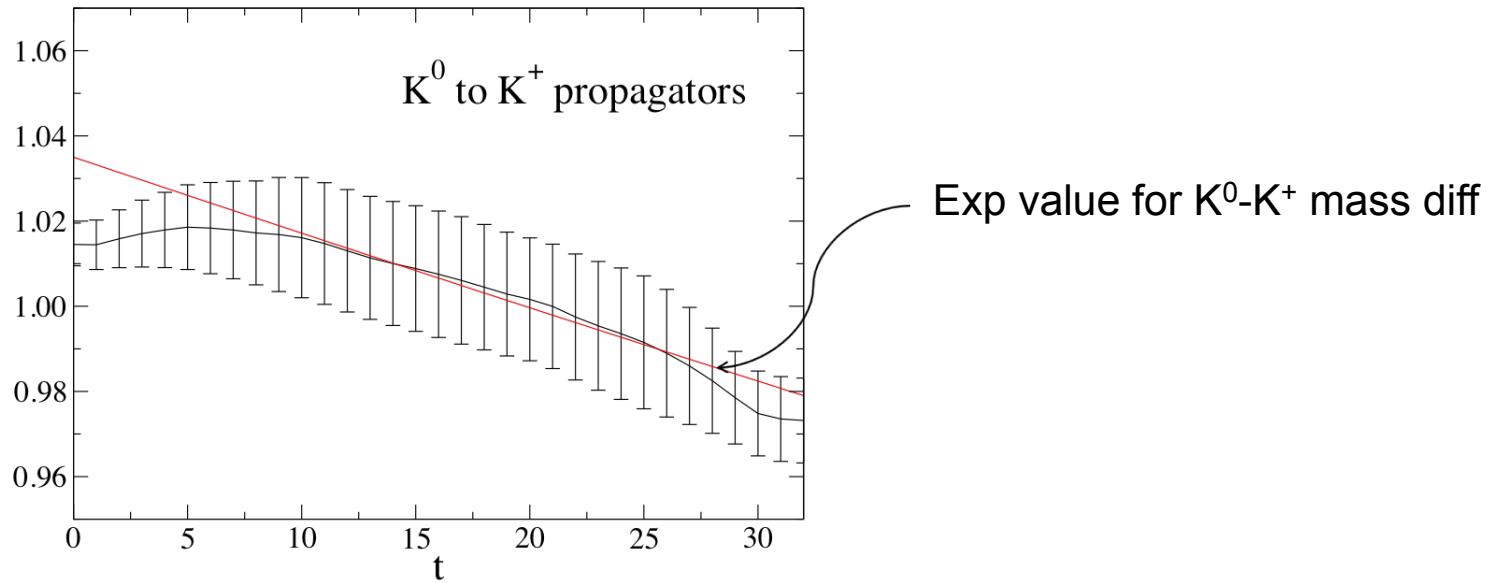
	Our results [MeV]	Experiment [MeV]
$m_{\pi^+}$	137.7(8.0)	139.57018(35)
$m_{K^+}$	492.3(4.7)	493.677(16)
$m_{K^0}$	497.4(3.7)	497.614(24)
$m_{\Omega^-}$	input	1672.45(29)



plateau close to the experimental value for  $N_\eta \geq 4$



## Ratio of $K^0$ to $K^+$ propagators



$$\frac{\langle K^0(t)K^0(0) \rangle}{\langle K^+(t)K^+(0) \rangle} \simeq Z \underbrace{(1 - (m_{K^0} - m_{K^+})t)}_{\text{much smaller than } 1}$$

much smaller than 1

Fit result  $4.54(1.09)$  MeV is consistent with exp value  $3.937(28)$  MeV



## Quark masses with NP renormalization factor

- NP renormalization factor with Schrödinger functional scheme  
PACS-CS, JHEP1008(2010)101

PRD81(2010)074503 [2+1f QCD (1)]  
PRD79(2009)034503 [2+1f QCD (2)]

- neglect QED corrections to the renormalization factor
- physical inputs:  $m_{\pi^+}$ ,  $m_{K^0}$ ,  $m_{K^+}$ ,  $m_{\Omega^-}$
- MS-bar scheme at  $\mu=2\text{GeV}$

	This work	2+1f QCD (1)	2+1f QCD (2)
$m_u$ [MeV]	2.57(26)(07)		
$m_d$ [MeV]	3.68(29)(10)		
$m_s$ [MeV]	83.60(58)(2.23)	86.7(2.3)	87.7(3.1)
$m_{ud}$ [MeV]	3.12(24)(08)	2.78(27)	3.05(12)
$m_u/m_d$	0.698(51)		
$m_s/m_{ud}$	26.8(2.0)	31.2(2.7)	28.78(40)

- possible QED finite size effects: -13.50% for u, +2.48% for d, -0.07% for s

Blum et al., PRD82(2010)094508



## §6. Summary

- 1+1+1 flavor QCD+QED simulation at the physical point
- Dynamical quark effects in QED and u-d quark mass difference are incorporated by reweighting technique
- u,d,s quark masses are determined with  $m_{\pi^+}$ ,  $m_{K^0}$ ,  $m_{K^+}$ ,  $m_{\Omega^-}$  as physical inputs
- Direct investigation of finite size effects due to QED is left as a future work